Photoemission and the Origin of High Temperature Superconductivity

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The condensation energy can be shown to be a moment of the change in the occupied part of the spectral function when going from the normal to the superconducting state. As a consequence, there is a one to one correspondence between the energy gain associated with forming the superconducting ground state, and the dramatic changes seen in angle resolved photoemission spectra. Some implications this observation has are offered.

In 1956, Chester published an interesting paper [1] which dealt with the the difference in energy between the normal and superconducting states (the condensation energy). For an isotope coefficient of one-half, he demonstrated that the condensation energy could be equated to the change in ion kinetic energy. Historically, the paper did not play a major role, since in the same year, the BCS theory of superconductivity was being developed, solving the problem of classical superconductors.

In this millenial year, though, we are faced with the unsolved problem of high T_c superconductivity. Because of this, several of us have invoked the name of Chester. The hope is that by directly focusing on the condensation energy, some light might be shed on the solution to the high T_c problem. This is particularly relevant if, as most of us suspect, the origin of high T_c is associated directly with electron-electron interactions. In such a case, treating the pair glue as an external object, as in the electron-phonon problem, could be misleading. In essence, the electrons are gluing themselves together. This indicates that new ways of thinking may be important.

This has led a number of authors to concentrate on the change in various response functions when going into the superconducting state. This is illustrated as follows:

$$\Delta \rightarrow G, F \rightarrow R \rightarrow F_N - F_S \rightarrow \Delta \qquad (1)$$

The idea is to assume a non-zero superconducting order parameter, Δ. This leads to changes in the normal Greens function, G, and to the creation of an anomalous Greens function, the Gor'kov F function. This in turn causes changes in various two-particle response functions, R: the dynamic spin susceptibility, the dielectric function, the optical conductivity, etc. This in turn leads to a change in the free energy between the normal (F_N) and superconducting (F_S) states. If the free energy is lowered, then a non-zero superconducting order parameter is self-consistently stabilized. Note that nowhere in this argument does the question of the pair glue arise. That is, superconductivity is generated simply if the response function change is such as to lower the free energy.

A number of theories with this philosophy have been advocated, each focusing on a different response function. One due to Anderson and coworkers suggests that the c-axis kinetic energy is lowered in the superconducting state [2]. This leads to a change in the c-axis optical conductivity, which has received some experimental support [3]. A different suggestion has been made in regards to the planar conductivity [4].

Turning to "potential energy" explanations, Leggett [5] has advocated that the energy savings comes from the density-density response function. Perhaps better known is the work of Scalapino and White [6], where a lowering of the exchange

energy is suggested based on a change in the spin-spin response function. This idea was then connected to the appearance below T_c of the neutron resonance mode by Demler and Zhang [7], which has also received experimental support [8]. In all of these cases, a particular part of the free energy is being singled out, with the connection being made via a two particle correlation function.

Here, a different approach is advocated [9]. This is illustrated as follows:

$$\Delta \rightarrow G \rightarrow F_N - F_S \rightarrow \Delta \quad (2)$$

Note the simplified nature of this diagram relative to the first one. This argumentation is based on the following relation: [10]

$$U_N - U_S = \sum_{\mathbf{k}} \int d\omega (\omega + \epsilon_k) f(\omega) \left[A_N(\mathbf{k}, \omega) - A_S(\mathbf{k}, \omega) \right] \quad (3)$$

where U_N (U_S) is the internal energy of the normal (superconducting) state, $A(\mathbf{k}, \omega)$ the single-particle spectral function, $f(\omega)$ the Fermi function, and ϵ_k the bare energy dispersion. Eq. 3 is based on a reduced (single-band) Hamiltonian with two particle interactions, and in principle can be generalized to the multi-band case by replacing the scalar quantities in this equation by matrices in reciprocal lattice space. It is easily demonstrated that this equation using the BCS reduced Hamiltonian generates the BCS condensation energy, $\frac{1}{2}N(0)\Delta^2$.

Note that the right hand side of Eq. 3 is a moment of the occupied part of the single-particle spectral function A (A^-). There are strong arguments that A^- is being measured by angle-resolved photoemission (ARPES) measurements in quasi-2D systems [11]. As a consequence, we see that the high T_c phenomenon is intimally connected with the dramatic change in the photoemission lineshape when going below T_c.

A useful decomposition, especially in regards to the various theories mentioned above, is to break the right hand side of Eq. 3 up into separate kinetic and potential energy pieces. This is easily implemented by rewriting $(\omega + \epsilon_k)$ as $(2\epsilon_k) + (\omega - \epsilon_k)$, the first term being the kinetic energy, the second the potential energy. Therefore, changes in the kinetic energy are associated with changes in the momentum distribution function (which is related to the integrated ARPES spectral weight [11]), whereas on the Fermi surface, the potential energy contribution reduces to the first moment of A^-.

This is easily illustrated for the case of BCS theory [12]. In this case, the potential energy is lowered by Δ^2/V, where V is the pair potential, and the kinetic energy increased by $\Delta^2/V - \frac{1}{2}N(0)\Delta^2$, the sum being the BCS condensation energy. The kinetic energy change is a consequence of the broadening of the momentum distribution function by the BCS coherence factors. The potential energy change is easily explained as well. It is due to the difference in ϵ and $E = \sqrt{\epsilon^2 + \Delta^2}$. On the Fermi surface, this difference is maximal, leading to a potential energy lowering of $\Delta/2$ (the factor of $\frac{1}{2}$ coming from the coherence factors). When integrated over ϵ, one then obtains Δ^2/V.

There are two interesting points about the BCS example. First, the transition is potential energy driven (physically, this occurs because the ion terms which actually drive the transition are absorbed into the effective potential of the reduced Hamiltonian). Second, the condensation energy is confined to the vicinity of the Fermi surface by the coherence factors. Note that although the ultraviolet cut-off (the Debye energy) enters the individual kinetic and potential energy terms, it drops out of the net term.

There are several reasons to believe that this BCS analogy may be misleading in the high T_c problem. First, it assumes the existence of quasiparticles. This can be contrasted with the high T_c case, where although quasiparticle peaks exist below T_c, they do not exist above [13]. That is, even though the superconducting state is almost certainly a (superfluid) Fermi liquid, the normal state appears to be a non Fermi liquid [14]. As a Fermi liquid does a better job of diagonalizing the kinetic energy than a non Fermi liquid, then one might conjecture that the kinetic energy is indeed lowered in the superconducting state despite the coherence factors. Note that this does not violate the considerations of Chester [9]. That is, although Chester [1] demonstrated that the potential energy of the electrons must be lowered

and the kinetic energy raised in the superconducting state, these refer to the potential and kinetic energy terms of the total Hamiltonian, not those of the reduced one. Therefore, there is nothing that prevents the kinetic energy of the reduced Hamiltonian from being lowered.

Second, the BCS condensation energy is confined to a narrow shell around the Fermi surface. For the electron-electron case, though, we can anticipate that the whole Brillouin zone could be affected. This is corroborated by ARPES spectra, which do show changes in the spectra even well away from the Fermi surface. Moreover, ARPES data are characterized by regions of the zone where the dispersion is weak. These same regions of the zone are associated with the anomalous pseudogap seen in underdoped cuprates. Thinking about these regions of the zone, even in the superconducting state, in terms of standard Fermi surface based concepts may be misleading.

Eq. 3 suggests that the best way to get a handle on these issues is by a detailed study of the change in the ARPES lineshape throughout the zone. One objection is that the number being sought is small. For instance, Loram, based on specific heat data, estimates the condensation energy to be only 3K per plane for optimal doped YBCO [15]. On the other hand, the relative contribution from a given **k** point is a different matter. As noted above, in BCS theory, **k** points on the Fermi surface yield a contribution to the condensation energy of $\Delta/2$, which is a substantial number.

A quick look at the data is sufficient to indicate potential pitfalls, along with suggestions about what may be going on. The $(\pi, 0)$ point is singled out since it exhibits the most dramatic lineshape change. In the normal state, one has an extremely broad spectral peak, with a width of order the entire bandwidth. In the superconducting state, this gets dramatically rearranged into a sharp spectral peak, followed at higher binding energy by a dip and hump. By comparing these two spectra, we get some idea about contributions of each spectral feature to the condensation energy.

We begin by looking at the first moment (ω) part of Eq. 3. There will be a positive contribution from the sharp spectral peak, which will be followed by a negative contribution from the spectral dip. Although the latter is smaller in weight than the former, it is enhanced because of the ω weighting. This is then followed by the hump and subsequent tail region, and therein lies the rub. Since this region is weighted by ω, it is sensitive to how the data are normalized. Typically, ARPES data are normalized in such a way that the high energy tails match, and thus to first approximation there is no tail contribution. But, if one assumes (on the Fermi surface) that the data are normalized by having equal integrated weight, then typically the tails do not quite match. The resulting tail contribution to Eq. 3 can be quite large. Similar considerations enter for the kinetic (ϵ_k) part of Eq. 3, where one deals with the change in integrated area. The message here is that since there are varying positive and negative contributions to the condensation energy from any given spectrum, then the normalization issue will have to be resolved before we can gain insight from Eq. 3 based on ARPES data.

Still, a qualitative statement can be made concerning the doping dependence of the condensation energy. It is now well known that the weight in the quasiparticle peak is dramatically suppressed as the doping is reduced [16]. In the context of Eq. 3, this implies a decrease in the condensation energy with underdoping. Moreover, since the normal state in the underdoped case is gapped, one expects a further reduction. These two observations go a long way in explaining the dramatic reduction in the condensation energy inferred from specific heat data [15].

To gain further insight, we have studied [9] the so-called mode model [17], developed to explain the lineshape change noted above. The idea is that the superconducting lineshape is very similar to that expected for electrons interacting with a collective mode. Detailed analysis of the data vs. doping [16] has verified that the mode is almost certainly the resonance mode observed by neutron scattering [8]. The model consists of a constant scattering rate (Γ) in the normal state, which becomes gapped in the superconducting state (this gap, which defines the spectral dip, is equal to $\Delta+\Omega_0$ where Ω_0 is the mode energy). Of

particular note, the quasiparticle peak is a consequence of a non-zero Ω_0.

The results for the condensation energy are surprising [9]. Near the Fermi surface, the kinetic energy is lowered, and the potential energy raised. The former occurs because the formation of quasiparticle peaks has a larger effect on sharpening the momentum distribution than the coherence factors have on broadening it. The potential energy lowering is a more subtle matter. The gap in ImΣ causes ReΣ by the Kramers-Kronig relation to have a logarithmic behavior. Because of this, the normal and superconducting state spectra only asymptotically approach one another. This leads to a large negative tail contribution to the first moment in Eq. 3, much larger than the positive contribution from the quasiparticle peak. As a result, the potential energy is raised. The kinetic energy driven nature of the transition is surprising, given the expectation that the neutron resonance mode should lead to a lowering of the exchange energy [7]. This behavior, though, is sensitive to the size of Γ. As Γ is reduced (the doping is increased), the normal state becomes more Fermi-liquid like, and one crosses over to the BCS limit, where the transition becomes potential energy driven.

This behavior is reminiscent of a phase diagram for the cuprates recently suggested by Phil Anderson [18]. The potential energy is lowered below a temperature T^* due to the formation of the pseudogap. This line merges with T_c on the overdoped side, and so the superconducting transition is potential energy driven on this side. On the underdoped side, though, the transition is kinetic energy driven, since the potential energy savings already occurs at T^*, and the additional kinetic energy savings is driven by quasiparticle formation. It is again important to note that despite the presence of a large spectral gap in the underdoped case, quasiparticle peak formation is still associated with T_c [19]. Also, this conjecture is consistent with Basov's results [3], in that the sum rule violation he reports (indicating a lowering of the kinetic energy) only occurs on the underdoped side of the phase diagram.

In conclusion, we suggest that Eq. 3 will be very useful when thinking about the origin of high T_c, and that ARPES data will play a major role in this endeavor.

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